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On critical stability of three quantum charges interacting through delta potentials

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Abstract

We consider three one dimensional quantum, charged and spinless particles interacting through delta potentials. We derive sufficient conditions which guarantee the existence of at least one bound state.

1 Introduction

Denote by $x_i, m_i, Z_i e$, $i = 1,2,3$, the position, mass and charge of the i-th particle. Our system is formally described by the Hamiltonian $\sum_{i=1}^{3} -\frac{\hbar^2}{2m_i}\partial_{x_i}^2 + \sum_{1\leq i<j\leq 3} Z_i Z_j e^2 \delta(x_i - x_j)$ acting in $L^2(\mathbb{R}^3)$ which is defined as the unique self-adjoint operator associated to the quadratic form with domain $\mathcal{H}^1(\mathbb{R}^3)$:

$$\sum_{i=1}^{3} \frac{\hbar^2}{2m_i}\|\partial_{x_i}\psi\|^2 + \sum_{1\leq i<j\leq 3} Z_i Z_j e^2 \int_{x_i=x_j} |\psi(\sigma_{i,j})|^2 d\sigma_{i,j}, \quad \psi \in \mathcal{H}^1(\mathbb{R}^3).$$

Here $\sigma_{i,j}$ denotes a point in the plane $x_i = x_j$. We will consider the cases $m_1 = m_2 =: m > 0$, $m_3 =: M > 0$ $Z_1 = Z_2 = -1$, $Z_3 =: Z > 0$ and answer to the question: *for what values of m/M and Z does this system possess at least one bound state after removing the center of the mass?*

There is a huge amount of literature on 1-d particles interacting through delta potentials either all repulsive or all attractive, but rather few papers deal with the mixed case. We mention the work of Rosenthal, [7], where he considered $M = \infty$. The aim of this paper is to make a systematic mathematical study of the Rosenthal results and extend them to the case $M < \infty$. It has been shown in [1] and [2] that these delta models serve as effective Hamiltonians for atoms in intense magnetic fields or quasi-particles in carbon nanotubes. As one can see in ([4], [5], [6],[3]), they also seem to be relevant for atomic wave guides, nano and leaky wires.

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$\frac{M}{m}$	$\theta_{2,3}$	$\theta_{1,2}$	α^2	$\nu(\alpha)$
1	$2\pi/3$	$2\pi/3$	$3/4$	1
∞	$3\pi/4$	$\pi/2$	$1/4$	$1/\sqrt{2}$

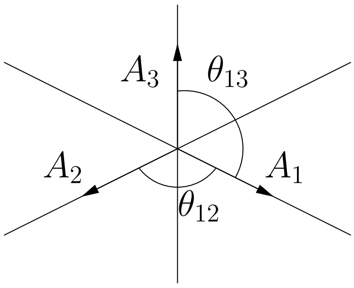

Figure 1: Left: table with corresponding values of angles and masses, right: support of the delta potentials with the unit vectors A_i's.

2 The spectral problem

Removing the center of mass. Using the Jacobi coordinates: $x := x_2 - x_1$, $y := x_3 - (m_1x_1 + m_2x_2)/(m_1+m_2)$ and $z := \sum_i m_i x_i / \sum_i m_i$ we get the 2-d relative motion formal Hamiltonian $\widetilde{H} = -\frac{\hbar^2}{m}\partial_x^2 - \frac{2m+M}{4mM}\hbar^2\partial_y^2 + e^2\delta(x) - Ze^2\delta(y - \frac{x}{2}) - Ze^2\delta(y + \frac{x}{2})$. Define $\alpha^2 := (M+2m)/4M$ and $\nu(\alpha) := \sqrt{1/4+\alpha^2}$. Let J be the Jacobian of the coordinate change $(x', y') = \{2\nu(\alpha)\hbar^2/(mZe^2)\}(x, \alpha y)$, and define the unitary $(U^{-1}f)(x,y) = \sqrt{J}f(x',y')$. Consider three unit vectors of $\mathbb{R}^2$ given by $A_1 := \frac{1}{\nu(\alpha)}\left(\alpha, -\frac{1}{2}\right)$, $A_2 := \frac{1}{\nu(\alpha)}\left(-\alpha, -\frac{1}{2}\right)$, and $A_3 := (0,1)$. Define $A_i^\perp$ as A_i rotated by $\pi/2$ in the positive sense. Then $U\widetilde{H}U^{-1} = \{mZ^2e^4\}/\{2\hbar^2\nu(\alpha)^2\}\ H$, where:

$$H := -\frac{1}{2}\partial_x^2 - \frac{1}{2}\partial_y^2 - \delta(A_1^\perp.(x,y)) - \delta(A_2^\perp.(x,y)) + \lambda\delta(A_3^\perp.(x,y)), \quad \lambda := \frac{\nu(\alpha)}{Z}.$$

We denote by $\theta_{i,j}$ the angle between the vectors A_i and A_j. We give some typical values of all these parameters (see fig. 1).

The skeleton Let A be unit vector in $\mathbb{R}^2$. If one introduce the "trace" operator $\tau_A : \mathcal{H}^1(\mathbb{R}^2) \to L^2(\mathbb{R})$ defined as $(\tau_A\psi)(s) := \psi(sA)$ and if we let $\tau : \mathcal{H}^1(\mathbb{R}^2) \to \bigoplus_{i=1}^3 L^2(\mathbb{R})$ be defined as $\tau := (\tau_{A_1}, \tau_{A_2}, \tau_{A_3})$, we may rewrite the Hamiltonian H as $H_0 + \tau^\star g\tau$ where $2H_0$ stands for the free Laplacian and g is the 3×3 diagonal matrix with entries $(-1,-1,\lambda)$. Denoting $R_0(z) := (H_0 - z)^{-1}$and $R(z) := (H-z)^{-1}$ the resolvents of H_0 and H, one derives at once, with the help of the second resolvent equation, the formula for any z in the resolvent sets of H_0 and H:

$$R(z) = R_0(z) - R_0(z)\tau^*(g^{-1} + \tau R_0(z)\tau^*)^{-1}\tau R_0(z). \tag{1}$$

Using the HVZ theorem (see [8] for the case with form-bounded interactions), we can easily compute the essential spectrum: $\sigma_{\rm ess}(H) = [-\frac{1}{2}, \infty)$. Its bottom is given by the infimum of the spectrum of the subsystem made by the positive charge and one negative charge.

¿From this and formula (1) it is standard to prove the following lemma:

Lemma 1. *Let $k > \frac{1}{\sqrt{2}}$. Define $\mathbf{S} := k\,g^{-1} + \tau R_0(-1)\tau^*$. Then $E = -k^2 < -\frac{1}{2}$ is a discrete eigenvalue of H if and only if* $\ker(g^{-1} + \tau R_0(E)\tau^*) \neq \{0\}$.

Note that up to a scaling this is the same as $\ker \mathbf{S} \neq \{0\}$. *Moreover,* $\mathrm{mult}(E) = \dim(\ker \mathbf{S})$.

The spectral analysis is thus reduced to the study of $\mathbf{S}$, a 3×3 matrix of integral operators each acting in $L^2(\mathbb{R})$. We call $\mathbf{S}$ the *skeleton* of H. Let us denote by $T_{A,B} := \tau_A R_0(-1)\tau_B^\star$, $T_0 := T_{A,A}$, by $\theta_{A,B}$ the angle between two unit vectors A and B, and by $\widehat{T}_{A,B}$ the Fourier image of $T_{A,B}$. Then the kernel of $\widehat{T}_{A,B}$ when $\theta_{A,B} \notin \{0, \pi\}$, and of $\widehat{T}_0$ read as:

$$\widehat{T}_{A,B}(p,q) = \frac{1}{2\pi|\sin(\theta_{A,B})|} \frac{1}{\left(\frac{p^2 - 2\cos(\theta_{A,B})pq + q^2}{2\sin^2(\theta_{A,B})} + 1\right)}, \quad \widehat{T}_0(p,q) = \frac{\delta(p-q)}{\sqrt{p^2+2}}. \tag{2}$$

Then $\widehat{T}_0$ is a bounded multiplication operator, and $\widehat{T}_{A,B}$ only depends on $|\theta_{A,B}|$. Consequently we denote in the sequel T_{A_i,A_j} by $T_{\theta_{i,j}}$ or $T_{i,j}$.

Reduction by symmetry. H and $\mathbf{S}$ enjoy various symmetry properties which follow from the fact that two particles are identical. Let $\pi : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the parity operator, i.e. $\{\pi\varphi\}(p) = \varphi(-p)$ and denote by $\pi_1 := \pi \otimes 1$ and $\pi_2 := 1 \otimes \pi$ the unitary symmetries with respect to the x and y axis. One verifies that for all $i, j \in \{1, 2\}$, we have $[\pi_i, H] = 0$ and $[\pi_i, \pi_j] = 0$. Thus if we denote by π_i^α, $\alpha = +, -$ the eigenprojectors of π_i on the even, respectively odd functions we may decompose H into the direct sum

$$H = \bigoplus_{\alpha\in\{\pm\},\, \beta\in\{\pm\}} H^{\alpha,\beta}, \quad H^{\alpha,\beta} := \pi_1^\alpha \pi_2^\beta H.$$

Similarly let $\Pi, \sigma : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ defined by $(\Pi\psi)(-p) := \psi(-p)$ and $\sigma\psi = \sigma(\psi_1, \psi_2, \psi_3) := (\psi_2, \psi_1, \psi_3)$. They both commute with $\mathbf{S}$, and also $[\Pi, \sigma] = 0$.

Let Π^α and σ^α, $\alpha = +, -$, denote the eigenprojectors of Π and σ symmetric and antisymmetric resp.. Then we can write $\mathbf{S} = \bigoplus_{\alpha\in\{\pm\},\, \beta\in\{\pm\}} \mathbf{S}^{\alpha,\beta}$, $\quad \mathbf{S}^{\alpha,\beta} := \Pi^\alpha \sigma^\beta \mathbf{S}$.

From the expression of $\widehat{T}_\theta(p,q)$ one also sees that $[\pi, T_\theta] = 0$ so that T_θ decomposes into $T_\theta^+ \oplus T_\theta^-$ where $T_\theta^\pm := \pi^\pm T_\theta$. As usual we shall consider $T_\theta^\pm$ as operators acting in $L^2(\mathbb{R}_+)$. Due to these symmetry properties we have $\ker \mathbf{S} = \bigoplus_{\alpha,\beta} \ker \mathbf{S}^{\alpha,\beta}$, and each individual null-space can be expressed as the null-space of a single operator acting in $L^2(\mathbb{R}_+)$ that we call *effective skeleton*. We gather in the following table the four effective skeletons we have to consider with their corresponding subspaces in $L^2(\mathbb{R}^2)$:

$S^{\alpha,\beta}$	effective skeleton	subspace in $L^2(\mathbb{R}^2)$
$++$	$k - T_0 - T_{1,2}^+ + 2T_{2,3}^+(T_0 + k\lambda^{-1})^{-1}T_{2,3}^+$	$\mathrm{Ran}\, \pi_1^+\pi_2^+$
$-+$	$k - T_0 - T_{1,2}^- + 2T_{2,3}^-(T_0 + k\lambda^{-1})^{-1}T_{2,3}^-$	$\mathrm{Ran}\, \pi_1^+\pi_2^-$
$+-$	$k - T_0 + T_{1,2}^+$	$\mathrm{Ran}\, \pi_1^-\pi_2^-$
$--$	$k - T_0 + T_{1,2}^-$	$\mathrm{Ran}\, \pi_1^-\pi_2^+$

Table 1.

3 Sectors without bound states

Properties of the T_θ operators. From (2) we get $0 \le T_0 \le 1/\sqrt{2}$. Then T_θ is self-adjoint and has a finite Hilbert-Schmidt norm. The proof of the following lemma in not at all obvious, but will be omitted due to the lack of space.

Lemma 2. *For all $\theta \in [\pi/2,\pi)$ one has $\pm T_\theta^\pm \geq 0$ and the mapping $[\pi/2,\pi) \ni \theta \mapsto \pm \inf T_\theta^\pm$ is strictly increasing.*

Absence of bound state in the odd sector with respect to y. We have the following result:

Theorem 3. *For all $Z > 0$ and all $0 < M/m \leq \infty$, H has no bound state in the symmetry sector* $\operatorname{Ran}\pi_2^-$.
Proof. The symmetry sector $\operatorname{Ran}\pi_2^-$ corresponds to the second and third lines in Table 1. For the third line one uses that $T_{1,2}^+ \geq 0$ by Lemma 2, and that $k > 1/\sqrt{2}$ since we are looking for eigenvalues below $\sigma_{\text{ess}}(H) = [-\frac{1}{2},\infty)$. Hence

$$k - T_0 + T_{1,2}^+ \geq k - \frac{1}{\sqrt{2}} > 0$$

thus $\ker(k - T_0 + T_{1,2}^+) = \{0\}$, and by Lemma 1 this shows that H has no eigenvalues in $\operatorname{Ran}\pi_1^-\pi_2^-$. By the same type of arguments one has: $k - T_0 - T_{1,2}^- + 2T_{2,3}^-(T_0 + k\lambda^{-1})^{-1}T_{2,3}^- \geq k - \frac{1}{\sqrt{2}} > 0$. ∎

Remark 4. The above theorem has a simple physical interpretation. Wave functions which are antisymmetric in the y variable are those for which the positive charge has a zero probability to be in the middle of the segment joining the negative charges. A situation which is obviously not favorable for having a bound state.

Absence of bound state in the odd-even sector with respect to x and y. Looking at the fourth line of Table 1 we have to consider

$$S^{-,-}(k) := k - T_0 + T_{1,2}^- =: \sqrt{k - T_0}\left(1 + \widetilde{T}_{1,2}^-(k)\right)\sqrt{k - T_0} \qquad (3)$$

where $\widetilde{T}_{1,2}^-(k) := (k - T_0)^{-\frac{1}{2}} T_{1,2}^-(k - T_0)^{-\frac{1}{2}}$. Here we will only consider the case $M \geq m$, i.e. $\pi/2 \leq \theta_{1,2} \leq 2\pi/3$. Assume that we can prove that $\widetilde{T}_{1,2}^-(2^{-\frac{1}{2}}) \geq -1$ for $\theta_{1,2} = 2\pi/3$, this will imply that $S^{-,-}(2^{-\frac{1}{2}}) \geq 0$ first for $\theta_{1,2} = 2\pi/3$ and then for all $\pi/2 \leq \theta_{1,2} \leq 2\pi/3$ by the monotonicity of $\inf T_{1,2}^-$ with respect to θ as stated in Lemma 2; finally looking at (3) this will show that $S^{-,-}(k) > 0$ for all $k > 1/\sqrt{2}$ and therefore that $\ker S^{-,-}(k) = \{0\}$. But $\widetilde{T}_{1,2}^- := T_{1,2}^-(2^{-\frac{1}{2}})$ (for $\theta_{1,2} = 2\pi/3$) is Hilbert-Schmidt since its kernel decay at infinity faster than the one of $T_{1,2}^-$ and it has the following behavior at the origin: $\widetilde{T}_{1,2}^-(p,q) \sim -\frac{16\sqrt{2}}{3\sqrt{3}\pi} + \mathcal{O}\left((p^2+q^2)\right)$. It turns out that -1 is an eigenvalue of $\widetilde{T}_{1,2}^-$ with eigenvector

$$\mathbb{R}_+ \ni p \mapsto \frac{\left[\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{p^2+2}}\right]^{1/2}}{p\,(2p^2+3)} \quad \overset{p\to 0}{\sim} \quad \frac{1}{3\,2^{\frac{5}{4}}} + \mathcal{O}(p^2)$$

and since the Hilbert-Schmidt norm of $\widetilde{T}_{1,2}$ can be evaluated numerically to $\|\widetilde{T}_{1,2}^-\|_{HS} \leq 1.02$, all the other eigenvalues of $\widetilde{T}_{1,2}^-$ are above -1. Thus we have proved the

Theorem 5. *For all $Z > 0$ and all $1 \leq M/m \leq \infty$, H has no bound state in the symmetry sector* $\operatorname{Ran}\pi_1^-\pi_2^-$.

4 The fully symmetric sector

According to Table 1, we need to find under which conditions one has $\ker S^{+,+}(k) \neq \{0\}$ where

$$S^{+,+}(k) := k - T_0 - K(k), \quad \text{with} \quad K(k) := T^{+}_{1,2} - 2T^{+}_{2,3}(T_0 + k\lambda^{-1})^{-1}T^{+}_{2,3}.$$

The proof of the following lemma is an easy application of Fredholm and analytic perturbation theory:

Lemma 6.(i) $\{\operatorname{Re} k^2 > 0\} \ni k \mapsto S^{+,+}(k)$ *is a bounded analytic self-adjoint family of operators.*
(ii) *If* $\inf \sigma \left(S^{+,+}(2^{-\frac{1}{2}}) \right) < 0$, *then there exists* $k > 1/\sqrt{2}$ *so that* $\ker S^{+,+}(k) \neq \{0\}$.

Denote by $\mathcal{K}(p,q)$ the integral kernel of $K(2^{-\frac{1}{2}})$. Our last result is:

Theorem 7. *For all* $0 < M/m \leq \infty$, *H has at least one bound state in the symmetry sector* $\operatorname{Ran} \pi_1^+ \pi_2^+$ *if Z is such that* $\mathcal{K}(0,0) > 0$.

Proof. We will now look for an upper bound on $\inf S^{+,+}(2^{-\frac{1}{2}})$ by the variational method. Let $j \in C_0^\infty(\mathbb{R}_+, \mathbb{R}_+)$ so that $\int_{\mathbb{R}_+} j(x)dx = 1$ and define two families of functions: $\forall \epsilon > 0,\ \psi_\epsilon(p) := \epsilon^{-1} j(p\epsilon^{-1}),\ \phi_\epsilon := \frac{\sqrt{\epsilon}}{\|j\|}\psi_\epsilon,\ \|\phi_\epsilon\| = 1$. We know that ψ_ϵ converges as $\epsilon \to 0$ to the Dirac distribution. First one has

$$\begin{aligned} ((2^{-\frac{1}{2}} - T_0)\phi_\epsilon, \phi_\epsilon) &= \frac{1}{\epsilon\sqrt{2}\|j\|^2} \int_{\mathbb{R}_+} [1 - (1 + p^2/2)^{-1/2}] j^2(p/\epsilon) dp \\ &\leq \frac{\epsilon^2}{2\sqrt{2}\|j\|^2} \int_{\mathbb{R}_+} p^2 j(p)^2 dp. \end{aligned} \tag{4}$$

Then one has $(K(2^{-\frac{1}{2}})\phi_\epsilon, \phi_\epsilon) = \frac{\epsilon}{\|j\|^2}(K(2^{-\frac{1}{2}})\psi_\epsilon, \psi_\epsilon) = \frac{\epsilon}{\|j\|^2}(\mathcal{K}(0,0) + \mathcal{O}(\epsilon))$ so that $(S^{+,+}(2^{-\frac{1}{2}})\phi_\epsilon, \phi_\epsilon) = 2^{-\frac{1}{2}} - (T_0\phi_\epsilon, \phi_\epsilon) - (K(2^{-\frac{1}{2}})\phi_\epsilon, \phi_\epsilon)$ will be negative for $\epsilon > 0$ small enough, provided $\mathcal{K}(0,0) > 0$. ∎

It is possible to compute $\mathcal{K}(0,0)$ analytically. It can be shown that there exists $Z_c^{\text{ub}}(M/m)$ such that for any Z larger than this value, we have $\mathcal{K}(0,0) > 0$. If we now define the critical Z as

$$Z_c(M/m) := \inf\{Z > 0,\ H = H(Z, M/m) \text{ has at least one bound state}\},$$

it follows from our last theorem that $Z_c(M/m) \leq Z_c^{\text{ub}}(M/m)$.

The curve $Z_c^{\text{ub}}(M/m)$ is plotted on figure 2, where we used $\theta_{1,2}$ instead of the ratio M/m.

Remarks 8. (a) Rosenthal found numerically $Z_c^{\text{ub}}(\frac{\pi}{2})$, i.e. Z_c^{ub} for $M = \infty$ to be 0.374903. With our analytical expression of $\mathcal{K}(0,0)$ we know this value to any arbitrary accuracy: $Z_c^{\text{ub}}(\frac{\pi}{2}) = 0.37490347747000593278...$
(b) The above curve shows that an arbitrarily small positive charge of mass $M < 0.48m$ can bind two electrons. However we believe that the exact critical curve will show that $M < m$ and $Z > 0$ is sufficient to bind these two electrons.

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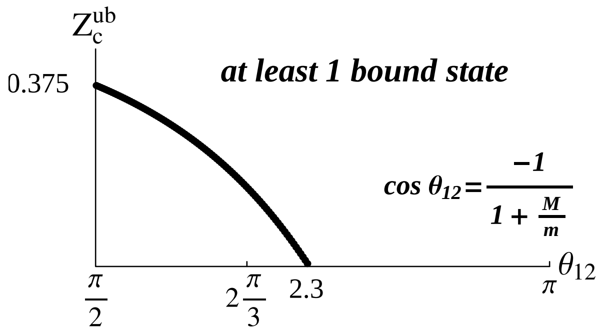

Figure 2: Graph of $Z_c^{\rm ub}$.

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References

[1] R. Brummelhuis, P. Duclos: Few-Body Systems **31**, 1-6, 2002

[2] Cornean H., Duclos P., Pedersen Th. G: Few-Body Systems **34**, 155-161, 2004

[3] P. Exner, T. Ichinose: J. Phys. **A34**(2001), 1439-1450

[4] K. Kanjilal, D. Blume: Phys. Rev. A **70** (2004), 042709

[5] Maxim Olshanii: Phys. Rev. Letters **81**(5) 1998, 938-941

[6] A.F. Slachmuylders, B. Partoens, W. Magnus, F.M. Peeters: Preprint cond-mat/0512385

[7] C.M. Rosenthal: Journ. Chem. Phys. **55**(5) 2474-2483 (1971)

[8] B. Simon: *Quantum mechanics for Hamiltonians defined as quadratic forms*. Princeton University press, New Jersey 1971